

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-
163702-07-6 | DTXSID4073120

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 34.2

Global applicability domain: Outside

Local applicability domain index: 2.65e-01

Confidence level: 6.50e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1,1,3,3,3-Hexafluoro-2-propanol</div> <div>Measured: 2.51</div> <div>Predicted: 2.40</div>	<div>Image not found</div> <div>Benzotrifluoride</div> <div>Measured: 44.7</div> <div>Predicted: 13.7</div>	<div>Image not found</div> <div>3-Chlorobenzotrifluoride</div> <div>Measured: 224</div> <div>Predicted: 317</div>
<div>Image not found</div> <div>2,4-Dichlorobenzotrifluoride</div> <div>Measured: 2340</div> <div>Predicted: 108</div>	<div>Image not found</div> <div>Dichlorodifluoromethane</div> <div>Measured: 6.17</div> <div>Predicted: 9.03</div>	